CURRENT RESEARCH AND DEVELOPMENT IN BIOTECHNOLOGY ENGINEERING AT IIUM

VOLUME II

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CHAPTER 28

IMPROVING ENZYME CATALYSIS THROUGH THE IMPROVEMENT OF BINDING STRENGTH: SIMULATED MUTATION TO PREDICT THE MUTATIONAL EFFECT ON XYLANASE CEX

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ABSTRACT

Xylanase enzymes are extensively used in biobleaching in the industry including paper and detergent industry. Hence the enhancement of their functional properties can give significant boost to this industry. Through this project, multiple trials have been conducted to suggest mutations to improve the properties of Xylanase enzyme family 10 from *Cellulomonas fimi*. The simulated mutation using Computer Aided Mutation (CAM) suggests enhancements in term of the binding strength that may lead to better catalysis reaction. The double point mutation of K47R and Q87N was found to increase binding of the ligands in the active site. Automated ligand docking analysis is used to demonstrate how different mutations can improve the binding strength of xylanase CeX. These results can be used to predict mutations that will improve the catalytic strength of the enzymes which can be used as a starting point for experimental studies.

Keywords: xylanase CeX, xylanase mutation, *Cellulomonas fimi,* computer aided design

INTRODUCTION

Xylanases are enzymes that catalyze the degradation of xylan, the main component of hemicellulose (Honda et al., 2091). Their biotechnological applications are of interest to the animal-feed, food-processing, and pulp-and-paper industries (Shibuya, 2000). In particular, xylanase has been found to be effective in reducing chlorine dosage requirements in the Kraft pulp-bleaching process (Viikari et al., 1994). Xylanase Cex is one of the xylanase enzymes from glycosyl hydrolase Family 10 (GH 10) (Davies, et al., 1995). It is from bacterium, Cellulomonas fimi and undergoes retaining mechanism. The active site nucleophile is Glu 233 (Tull et al., 1991) and the acid base catalyst is Glu 127 (MacLeod, 1994). In term of economical overview, for example in pulp industries (Suurnaki, 1996), the use of xylanase to degrade xylan is more beneficial compared to use of chemical processes which are expensive and cause environmental